

The Spectrum of the Fractional Laplacian and First Passage Time Statistics

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PACS 05.40.Fb – Random walks and Lévy flights

PACS 02.50.-r – Probability theory, stochastic processes, and statistics

PACS 89.65.Gh – Economics; econophysics, financial markets, business and management

Abstract. - We present exact results for the spectrum of the fractional Laplacian in a bounded domain and apply them to First Passage Time (FPT) Statistics of Lévy flights. We specifically show that the average is insufficient to describe the distribution of FPT, although it is the only quantity available in the existing literature. In particular, we show that the FPT distribution is not peaked around the average, and that knowledge of the whole distribution is necessary to describe this phenomenon. For this purpose, we provide an efficient method to calculate higher order cumulants and the whole distribution.

Anomalous diffusion is a widely investigated phenomenon with an increasing number of applications in natural sciences [1–6]. Stochastic Lévy processes serve as a paradigm for many unusual transport phenomena in which collective dynamics, extended heterogeneities and other sources of jumps with a long-range distribution play an important role and lead to anomalous diffusion. Lévy flights are governed by rare yet extremely large jumps of diffusing particles. In the continuous limit, which interests us here, the Lévy flight process is described by a fractional diffusion equation for the Lévy flyer concentration field $C(x, t)$, given by

$$\partial_t C(x, t) = -(-\Delta)^N C(x, t), \quad 0 < N < 1, \quad (1)$$

where $(-\Delta)^N$ is the Riesz-Feller derivative of fractional order $2N$, namely $(-\Delta)^N = \frac{\partial^{2N}}{\partial |x|^{2N}}$ [7]. Eq. (1) describes a diffusive process that is faster than normal diffusion (super-diffusive) [1], where the index N characterizes the degree of fractality of the environment. For $N > 1$ there is no probabilistic interpretation of the equation as a diffusion equation, although for various values of N Eq. (1) can have a different physical interpretation. For example, $N = 2$ corresponds to the overdamped vibrations of a flexible rod, or to the out-of-equilibrium fluctuations of a slowly growing film in molecular beam epitaxy [8].

Eq. (1) has to be supplemented with appropriate Boundary Conditions (BC) encoding the properties of the boundaries, such as absorbing boundary conditions

$$(-\Delta)^\mu C(\pm 1, t) = 0, \quad 0 \leq \mu < N/2. \quad (2)$$

Note that this condition should hold for all real values of μ in the interval $0 \leq \mu < N/2$. Although we will be interested here in the case $0 < N < 1$, it turns out useful to consider this equation more generally for any N , and to specialize to the desired range when drawing physical conclusions.

In the context of Lévy flights, a classical quantity of interest in such systems is the Mean First Passage Time (MFPT) defined as the average time needed for a stochastically moving particle to reach one of the two absorbing boundaries $x = \pm 1$, when it was initially located at some point x_0 in the interval. It can be shown [9] that the First Passage Time (FPT) distribution for the one dimensional bounded domain Ω with absorbing BC is obtained as

$$\rho(t|x_0) = -\frac{\partial}{\partial t} \int_{\Omega} C(x, t|x_0) dx, \quad (3)$$

where the notation includes x_0 giving explicit reference to the initial condition $C(x, 0|x_0) = \delta(x - x_0)$. In particular, moments of the distribution $\rho(t|x_0)$ are given by

$$\langle t^m \rangle(x_0) = \int_0^{\infty} t^m \rho(t|x_0) dt. \quad (4)$$

The MFPT in the presence of two absorbing boundaries can be exactly calculated using Sonin inversion formula [10], resulting in

$$\langle t \rangle(x_0) = \frac{(1 - x_0^2)^N}{\Gamma(2N + 1)}, \quad (5)$$

where $\Gamma(x)$ is Euler's Gamma function. This problem has been further studied both analytically and numerically; generalized to other boundary conditions [11, 12], to semi-infinite domains [13], and even to complex media [14].

A general question regarding the average is whether it is also representative. A simple test is to compare the average to the standard deviation of the distribution, or more generally to higher order cumulants. However, so far no attention has been given to the variance and other higher order moments of the distribution $\rho(t|x_0)$ of FPT for Lévy flights. Indeed, if the distribution is peaked around the average, then knowing the average gives a fair information about the process. This is exactly the case for the Gaussian distribution where the average and the variance summarizes completely the information about the distribution. However if the distribution is not Gaussian, the knowledge of higher order cumulants is important to characterize the process.

In the following we show that indeed the MFPT of Lévy flights is far from being representative, and knowledge of higher order moments, or actually the whole distribution, is needed to give a proper description of the statistics of FPT. In order to achieve this task, we start by obtaining detailed knowledge about the spectrum of the fractional Laplacian. Using analytical and numerical results of the spectrum, we then show that higher order moments are important in comparison to MFPT, especially in the vicinity of the absorbing boundaries. We also obtain the whole distribution of FPT. Finally, we comment on how this approach can be generalized to other boundary conditions, such as reflecting or mixed ones.

Fractional Laplacian in Bounded Domains. — In a recent paper [15] we developed an approach to study the spectrum of large powers of the Laplacian in bounded domains, continuing a previous effort [16] which focused on the ground state (i.e., the eigenfunction corresponding to the lowest eigenvalue). We showed that in the large N -limit the eigenfunctions of $(-\Delta)^N$ with absorbing BC are simply proportional to the associated Legendre polynomials $P_{2N+j}^{2N}(x)$ for $j \in \mathbb{N}$, and we showed how to obtain systematic corrections in powers of $1/N$. It turns out that this asymptotic expansion shows remarkable convergence, so that already for $N = 1$ the asymptotic spectrum is very close to the exact one. In addition, we showed that expressing $(-\Delta)^N$ in the basis of the associated Legendre polynomials does not only diagonalize it for $N \rightarrow \infty$, but is also a very useful basis for numerically evaluating its spectrum for any N . However, these results were limited to integer N 's and

are therefore inapplicable to the phenomena which interests us here, namely of anomalous diffusion.

Here we show how to extend the method developed in [15] to non-integer N 's. The challenge is to find an appropriate basis that satisfies the BC (2), and coincides with the associated Legendre polynomials for integer N 's. The following normalized functions form the required basis

$$f_j(x) = \frac{\Gamma(4N+1)\sqrt{(2j)!(2N+2j+\frac{1}{2})(1-x^2)^N}}{4^N\Gamma(2N+1)\sqrt{\Gamma(4N+2j+1)}}C_{2j}^{(2N+\frac{1}{2})}(x), \quad (6)$$

for $j \in \mathbb{N}$ (including $j = 0$), and $C_k^{(\lambda)}(x)$ are the Gegenbauer polynomials [17]. In order to show this, we need to write the matrix elements of the operator $(-\Delta)^N$ in this basis, namely

$$\hat{\Delta}_{m,j}^N \equiv \int_{-1}^1 f_m(x) [(-\Delta)^N f_j(x)] dx = \hat{\Delta}_{j,m}^N. \quad (7)$$

This can be achieved using $\frac{d^\mu}{d|x|^\mu}x^\lambda = \frac{\Gamma(\lambda+1)}{\Gamma(\lambda-\mu+1)}x^{\lambda-\mu}$ [7], and the series expansion of the Gegenbauer polynomials [17]

$$C_{2j}^{(\lambda)}(x) = \sum_{\ell=0}^j \frac{(-1)^\ell (\lambda)_{2j-\ell} (2x)^{2j-2\ell}}{\ell! (2j-2\ell)!}, \quad (8)$$

where $(\lambda)_n$ is the Pochhammer symbol. After some algebra similar to [15], the following expression for the matrix elements are obtained

$$\begin{aligned} \hat{\Delta}_{m,j}^N = & \sqrt{\frac{(2j)!(4N+2m)!}{(2m)!(4N+2j)!}} \sqrt{\frac{(4N+4m+1)(4N+4j+1)(-1)^{N+j}}{2^{2N+1}\Gamma(N+\frac{1}{2})}} \sum_{i=0}^j \frac{(-4)^i (2N+2i)! \Gamma(2N+j+i+\frac{1}{2}) \Gamma(i+\frac{1}{2})}{[(2i)!]^2 (j-i)! \Gamma(N+i+\frac{3}{2})} \\ & \times {}_3F_2 \left(\begin{matrix} i-j, -N, 2N+i+j+\frac{1}{2} \\ i+\frac{1}{2}, i+1 \end{matrix} ; 1 \right) {}_3F_2 \left(\begin{matrix} 2N+m+\frac{1}{2}, -m, N+1 \\ 2N+1, N+i+\frac{3}{2} \end{matrix} ; 1 \right) \end{aligned}, \quad (9)$$

where ${}_3F_2 \left(\begin{matrix} a, b, c \\ d, e \end{matrix} ; x \right)$ is the generalized hypergeometric function [17]. Interestingly, for integer N 's this expression coincides with the one obtained in [15]. This implies immediately that all the results obtained for large N 's apply also for the fractional case, and we can readily use the approach developed in [15] with the important difference that for non-integer N 's one should use as basis the functions (6) and not the associated Legendre polynomials. We therefore obtain for the eigenfunctions

$$\begin{aligned} v_j(x) = & f_j(x) + \frac{[(2j)(2j-1)]^{3/2}}{32N^2} f_{j-1}(x) \\ & - \frac{[(2j+2)(2j+1)]^{3/2}}{32N^2} f_{j+1}(x) + O\left(\frac{1}{N^3}\right), \end{aligned} \quad (10)$$

and for the eigenvalues

$$\begin{aligned} \lambda_j = & \sqrt{2} \frac{(4N)^{2j}}{(2j)!} \Gamma(2N+1) \left[1 - \frac{3+4j+8j^2}{16N} + \right. \\ & \left. + \frac{75+344j+672j^2+832j^3+192j^4}{1536N^2} + O\left(\frac{1}{N^3}\right) \right]. \end{aligned} \quad (11)$$

In particular, the numerical scheme of [15] will allow us to calculate to arbitrary precision all the quantities of interest, and thus provides a reference to the analytical results we present

below. Since we are interested in anomalous diffusion and thus primarily on small values of N , we will focus from now on only on the case $0 < N \leq 1$. To demonstrate that the numerical scheme of [15] can be extended to noninteger as well as small N 's, we present in Fig. 1 the first three eigenvalues $\lambda_0(N), \lambda_1(N), \lambda_2(N)$ in the range $0 \leq N \leq 1$. As can be seen, the lowest eigenvalue $\lambda_0(N)$ becomes smaller than one for values of $N \gtrsim 0.32$.

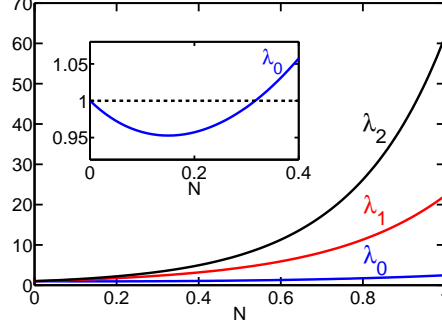


Fig. 1: The first three eigenvalues $\lambda_0(N), \lambda_1(N)$ and $\lambda_2(N)$ of $(-\Delta)^N$ in the range $0 \leq N \leq 1$. Note that all the eigenvalues are degenerate at $N = 0$ where their value is 1, and that only λ_0 becomes smaller than one in a certain range of N (see inset).

In the same line of [15] where a $1/N$ expansion has been performed, we begin by studying the small N behaviour of the operator $(-\Delta)^N$. To zeroth order in N , it is easy to show that Eq. (9) yields $\hat{\Delta}_{m,j}^N = \delta_{mj} + O(N)$, which is consistent with the simple fact that $(-\Delta)^0 = 1$. Going beyond zeroth order is cumbersome, and is mainly due to the expansion of the Generalized Hypergeometric functions. However, we have previously shown that (see appendix B in Ref. [15])

$$\begin{aligned}
{}_3F_2 \left(\begin{matrix} 2N+m+\frac{1}{2}, -m, N+1 \\ 2N+1, N+i+\frac{3}{2} \end{matrix} ; 1 \right) &= \sum_{\ell=0}^m \frac{j!}{\ell!(m-\ell)!} \frac{B(2N+m+\ell+\frac{1}{2}, \frac{1}{2}-\ell)}{B(2N+m+\frac{1}{2}, \frac{1}{2}-m)} \frac{B(N+1, i+\ell+\frac{1}{2})}{B(N+1, i+\frac{1}{2})} {}_4F_2 \\
{}_3F_2 \left(\begin{matrix} i-j, -N, 2N+i+j+\frac{1}{2} \\ i+\frac{1}{2}, i+1 \end{matrix} ; 1 \right) &= \frac{4^{-2N-j-i} \sqrt{\pi} (2i)!(j-i)!}{\Gamma(2N+j+i+\frac{1}{2})} \\
&\times \sum_{m=0}^{j-i} \frac{(4N+2j+2m+2i)!}{(2m+2i)!(j-m-i)!(2N+j+m+i)!} \frac{N!}{m!(N-m)!}, \quad (13)
\end{aligned}$$

where $B(x, y)$ is the Beta function. These representations render the small N expansion straightforward yet tedious. Then, the expansion of $\hat{\Delta}_{m,j}^N$ up to first order in N is given by

$$\hat{\Delta}_{m,j}^N = \delta_{mj} + N B_{m,j} + O(N^2), \quad (14)$$

with

$$B_{m,j} = \begin{cases} D_j, & m = j \\ \frac{\sqrt{(4m+1)(4j+1)}}{|m(2m+1)-j(2j+1)|}, & m \neq j \end{cases}, \quad (15)$$

and

$$\begin{aligned}
D_j &\equiv 4\psi_0(4j) - 4\psi_0(2j) - \frac{1}{j(4j+1)} - 2\gamma \\
&+ \frac{4j+1}{2\pi} \sum_{i=0}^j \frac{(-4)^i \Gamma(j+i+\frac{1}{2})}{(2i)!(j-i)!} \sum_{\ell=0}^j \frac{(-4)^\ell \Gamma(\ell+j+\frac{1}{2})}{(2\ell)!(j-\ell)!} \frac{[\gamma - \psi_0(i+\ell+\frac{3}{2}) + 2\psi_0(j+\ell+\frac{1}{2})]}{(\ell+i+\frac{1}{2})}, \quad (16)
\end{aligned}$$

Table 1: The first eigenvalues of the matrix B given by Eq. (15) - denoted b_j . Note that the lowest eigenvalue is negative ($b_0 < 0$), while all the rest are positive ($b_{j \geq 1} > 0$).

j	0	1	2	3	4	5
b_j	-0.688	2.727	3.909	4.646	5.183	5.606

where $\psi_0(x)$ is the digamma function and γ is the Euler-Mascheroni constant [17]. Note that D_0 is obtained by taking the limit $j \rightarrow 0$ in Eq. (16), namely

$$D_0 = 2(1 - \gamma - \ln 2) \simeq -0.541. \quad (17)$$

Equations (15-17) allow determining the eigenvalues and the eigenfunctions of the fractional Laplacian for small N . Note that the zeroth order term in the expansion of $(-\Delta)^N$ is just the identity, implying that at the lowest order, the eigenvalues are completely degenerate. This means that diagonalizing $(-\Delta)^N$ to first order is equivalent to the diagonalization of the matrix B given by Eq. (15). Once the eigenvalues $\{b_j\}$ and eigenvectors $\{\vec{\beta}_j\}$ of the matrix B are computed numerically, the eigenvalues $\{\lambda_j^B\}$ and eigenfunctions $\{v_j^B(x)\}$ of $(-\Delta)^N$ for small N follows immediately and are just given by

$$\lambda_j^B = 1 + N b_j, \quad (18)$$

$$v_j^B(x) = \sum_{n=0}^{\infty} \beta_j^{(n)} f_n(x), \quad (19)$$

where $\beta_j^{(n)}$ is the n^{th} component of $\vec{\beta}_j$. Notice that at this order, the N -dependence of $v_j^B(x)$ comes in only through the basis functions $f_n(x)$.

In Table 1, we provide the first eigenvalues of $B_{m,j}$. Interestingly, only the smallest eigenvalue b_0 is negative, implying that $\lambda_0^B < 1$, consistent with the numerical results presented in Fig. 1. The other eigenvalues $b_{j \geq 1}$ are all positive. This is in contradiction with the small N expression developed in [12] for the lowest eigenvalue, predicting $\lambda_0 = 1 + 2N(1 - \gamma) > 1$ (Eq. (36) there). The reason for this difference is twofold. First, in [12] the operator $(-\Delta)^N$ has been written using a trigonometric basis yielding a different first-order matrix $B_{m,j}$. For example, in the present notation, the value of D_0 obtained by [12] is $D_0^{ZRK} = 2(1 - \gamma) \simeq 0.846$. Second, the matrix $B_{m,j}$ has not been fully diagonalized in [12], but rather approximated by $\lambda_0 = 1 + N D_0^{ZRK}$, predicting a positive correction for λ_0 for small N 's. This suggests that the trigonometric basis used in [12] is not adequate for a perturbative analysis. Effectively, if we use the same approximation $\lambda_0 = 1 + N D_0$ we would obtain a negative correction, implying that the basis $\{f_j(x)\}$ is more adapted to the operator $(-\Delta)^N$. Note that the fact that the lowest eigenvalue is smaller than one can have important consequences regarding the stability of the process described by the fractional Laplacian. To allow for a more advanced comparison, we also show in Fig. 2 the ground state $v_0^B(x)$ obtained using this approximation, compared to the exact ground state $v_0(x)$ computed numerically from the diagonalization of (9), for various small values of N .

Complementary to the large- N study of Ref. [15] and the small- N study presented above, we now develop a useful approach for obtaining the ground state directly from the matrix $\hat{\Delta}_{i,j}^N$, without expanding around a particular value of N . Often in physical problems the ground state is the most interesting quantity, as will be shown to be the case for FPT too. For this purpose, we approximate the matrix $\hat{\Delta}_{m,j}^N$ as given by Eq. (9) so that the lowest eigenvalue is given by diagonalizing its upper 2×2 sub-matrix. We then find for the ground

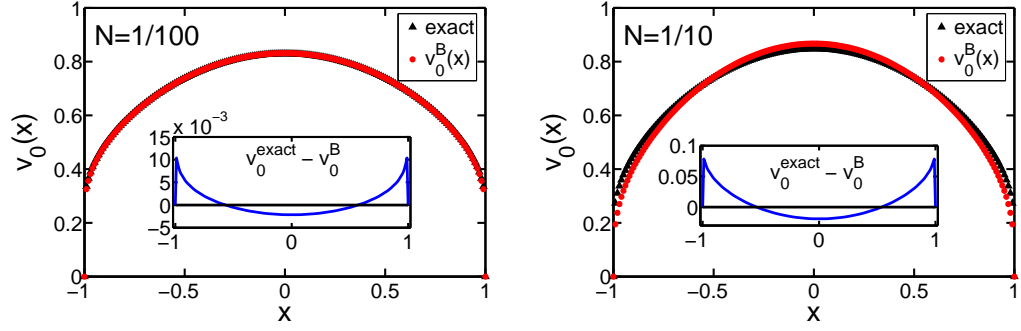


Fig. 2: A comparison of the exact ground state $v_0^{exact}(x)$ with $v_0^B(x)$ for various low values of N . The Insets show the difference $v_0^{exact}(x) - v_0^B(x)$.

state

$$\lambda_0^{2 \times 2}(N) = \frac{\Gamma(N) \Gamma(N+1) \Gamma(4N+2)}{2^{2N+1} \Gamma(2N) \Gamma(2N+2)} ab, \quad (20)$$

$$v_0^{2 \times 2}(x) = [f_0(x) + a f_1(x)] / \sqrt{1+a^2}, \quad (21)$$

where

$$\begin{aligned} a &= \left[(c+1) - \sqrt{(c-1)^2 + 4b^2} \right] / 2b, \\ b &= \frac{N}{2N+3} \sqrt{\frac{4N+5}{2N+1}}, \\ c &= \frac{(4N+5)(16N^4 + 40N^3 + 42N^2 + 18N + 3)}{(2N+1)(2N+3)(2N+5)}. \end{aligned} \quad (22)$$

As can be seen in Figs. 3-4, these expressions compare well with the exact numerical diagonalization of $\hat{\Delta}_{m,j}^N$.

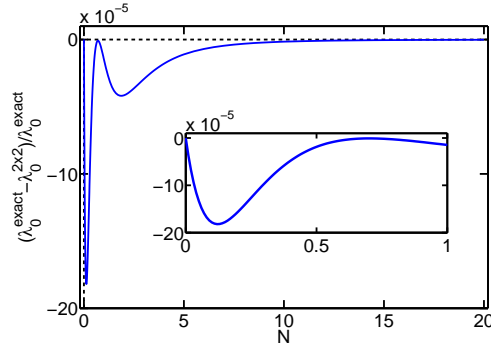


Fig. 3: A comparison of the smallest eigenvalue λ_0^{exact} with $\lambda_0^{2 \times 2}$ resulting from the 2×2 approximation for various values of N . Note that the relative error is always smaller than $2 \cdot 10^{-4}$ (see Inset) and that $\lambda_0^{2 \times 2}$ becomes exact when $N \rightarrow \infty$ [15].

First Passage Times. — Equipped with the new results concerning the spectrum of the fractional Laplacian, we can readdress the statistics of FPT of Lévy flights. It is easy to solve formally Eq. (1) as

$$C(x, t|x_0) = \sum_{j=0}^{\infty} e^{-\lambda_j(N)t} v_j(x) v_j(x_0), \quad (23)$$

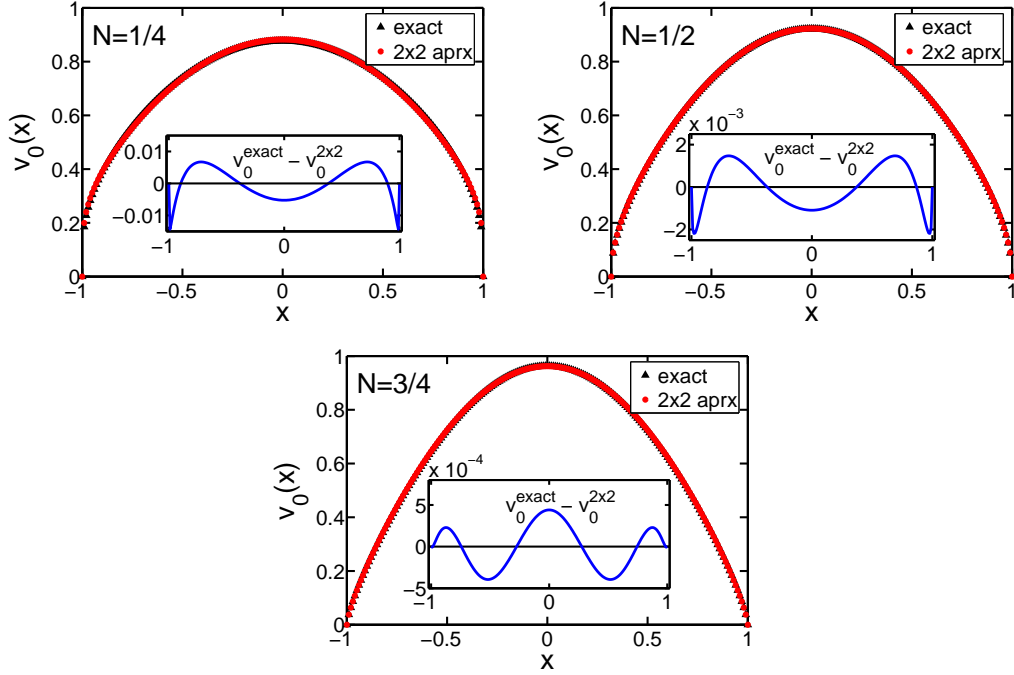


Fig. 4: A comparison of the exact ground state $v_0^{\text{exact}}(x)$ with $v_0^{2 \times 2}(x)$ resulting from the 2×2 approximation for various values of N . The Insets show the difference $v_0^{\text{exact}}(x) - v_0^{2 \times 2}(x)$.

where here too $\{v_j(x)\}$ are the eigenfunctions of $(-\Delta)^N$. Using Eq. (3) we obtain

$$\rho(t|x_0) = \sum_{j=0}^{\infty} \left(\int_{-1}^1 v_j(x) dx \right) \lambda_j(N) v_j(x_0) e^{-\lambda_j(N)t}, \quad (24)$$

and Eq. (4) for the moments becomes

$$\langle t^m \rangle(x_0) = \Gamma(m+1) \sum_{j=0}^{\infty} \frac{\left(\int_{-1}^1 v_j(x) dx \right)}{[\lambda_j(N)]^m} v_j(x_0). \quad (25)$$

We calculated numerically the moments using both Eq. (25) and a direct numerical diagonalization of $(-\Delta)^N$ as given by Eq. (9). In Fig. 5, we present the cumulants of the distribution $\kappa_m(x_0)$ for $N = 1/4, 1/2, 3/4$. Recall that the cumulants κ_m are simple combinations of $\langle t^m \rangle$ [17], and that for $m = 1, 2$ they coincide with the mean and the variance respectively. We also present results obtained using only the first term in Eq. (25), namely the ground state, which we calculate here using the 2×2 approximation (20,21). As can be seen in Fig. 5 the agreement between the two approaches is very good. This means that knowledge of the ground state provides a reasonable description of the distribution. Note that the cumulants grow faster as the value of N decreases.

However, these results show that $\kappa_m^{1/m}$ increases with m for all values of x_0 , implying that the mean $\langle t \rangle \equiv \kappa_1$ is generically not representative, since the distribution is not peaked around it. In that case the variance, and other higher order cumulants, are necessary to characterize the full distribution. Put differently, statistical inference regarding first passage properties based only on the mean can lead to wrong conclusions since the errors bars, calculated using the higher order moments, are typically larger than the the mean value itself. Last, Fig. 6 shows the full distribution of FPT, $\rho(t|x_0)$, for $N = 1/2$, calculated using

Eq. (24) and a straightforward application of the numerical scheme presented above. For long times $t \gg 1$ the tail of $\rho(t|x_0)$ is always exponential, and the lowest eigenvalue $\lambda_0(N)$ controls its decay rate. However, for short times, many terms has to be retained in the sum (24) giving rise to a nontrivial form.

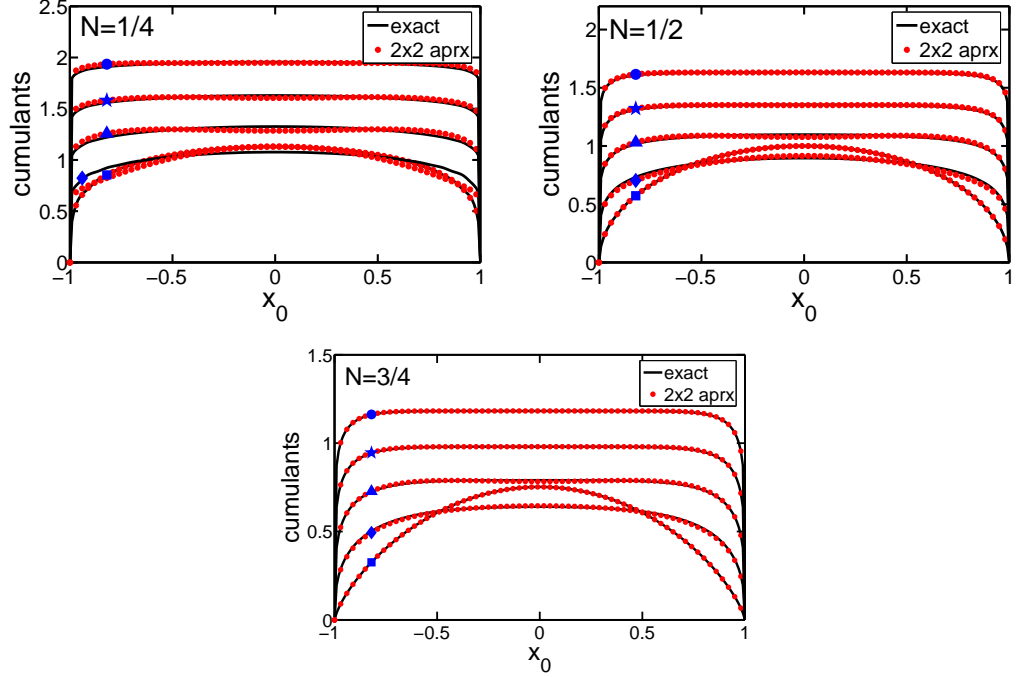


Fig. 5: A comparison of the first five cumulants as function of x_0 between the exact numerical result and the 2×2 approach for $N = 1/4$, $N = 1/2$ and $N = 3/4$. The symbols \blacksquare , \blacklozenge , \blacktriangle , \star , and \bullet correspond to $\langle t \rangle$, $\kappa_2^{1/2}$, $\kappa_3^{1/3}$, $\kappa_4^{1/4}$ and $\kappa_5^{1/5}$ respectively.

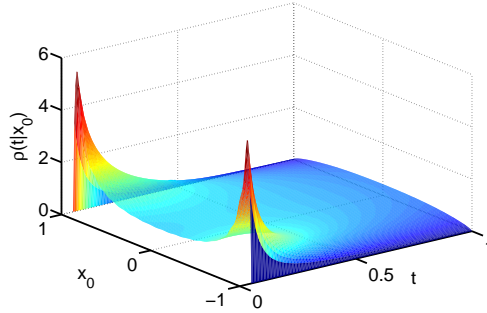


Fig. 6: The distribution of FPT $\rho(t|x_0)$ as a function of x_0 and t for $N = 1/2$.

Summary and discussion. — In this letter we obtain both analytical and numerical information about the spectrum of the fractional Laplacian in bounded domains, extending previous results for integer powers of the Laplacian [15]. These results allow us to address the timely question of FPT statistics. We show that in general the mean first passage time does not provide a proper description of the FPT distribution since the variance (as well as higher order cumulants) become more and more important as the Lévy stability index N

becomes smaller (see Fig. 5). This means that the distribution is not peaked around the average, as often implied when only the average is discussed. Therefore, the MFPT is not representative of the distribution, and the whole distribution $\rho(t|x_0)$ has to be retained. A direct consequence of these results is that the distribution of FPT is not Gaussian, contrarily to what is implicitly assumed when focussing on the average (MFPT) only. We show how to obtain the FPT distribution numerically for any N . In addition we show that a simple “ 2×2 ” approximation is able to reproduce accurately the cumulants. Our results (24) suggest that the tail of the distribution is exponential, while for short times it has a complex nontrivial form.

An interesting point, is that the lowest eigenvalue λ_0 becomes smaller than one (see the inset in Fig. 1) in a whole range of small N 's. Even though this result does not affect the FPT statistics studied here, this might have important consequences in systems described by the Fractional Laplacian, whose stability is determined by large powers of the eigenvalue of the ground state (an example of such a system can be found in [18]). Our result suggests that in such cases tuning the value of N (by changing the fractality of the medium for example) can control the stability of the system.

Note that we were interested above only in the even part of the spectrum of $(-\Delta)^N$ (that is the even eigenfunctions). The reason is that for the statistics of FPT with two absorbing boundaries we need to know only the even spectrum since the odd eigenfunction do not contribute to the expression for $\rho(t|x_0)$ as given by Eq. (24) due to the integral there. However, information about the odd spectrum can be easily obtained by replacing $j \rightarrow (j + 1/2)$ in Eqs. (6–16).

Last, we comment on how to treat other boundary conditions, such as reflecting or mixed ones [11]. The key observation is that one has $C_j^{(2N+\frac{1}{2})}(x) = P_j^{(2N,2N)}(x)$ where $P_j^{(\mu,\nu)}(x)$ is the j^{th} Jacobi polynomial [17]. Using orthogonality properties and BC of this polynomials it can be shown that the relevant basis for mixed BC (i.e., one reflecting and one absorbing boundary) is proportional to $\left\{ (1+x)^N (1-x)^{N+1} P_j^{(2N,2N+2)}(x) \right\}$.

Acknowledgements.—This work was supported by EEC PatForm Marie Curie action (E.K.). Laboratoire de Physique Statistique is associated with Universities Paris VI and Paris VII.

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